

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
S23	95	(568/902).CCLS.	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:02
S24	95	568/902.ccls.	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:28
S25	11	S24 and (propanediol or 3-propanediol or diol)	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:03
S26	328	568/678	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:31
S27	23	568/678.ccls. and propanediol	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:31

FILE 'BEILSTEIN' ENTERED AT 17:53:37 ON 15 APR 2004

L3 STRUCTURE UPLOADED  
L4 617733 S 2/O NOT N/ELS  
L5 526528 S L4 NOT (S/ELS OR X/ELS OR M/ELS)  
L6 526528 S L5 NOT PMS/CI  
L7 46 S L3 SUB=L5 FULL  
L8 0 S L7 AND 1-5/NR  
L9 8 S L7 AND PHENY?  
L10 38 S L7 NOT L9  
L11 2 S L10 AND (ISOPRO? OR METHYLETHYL OR TERTIARY BUTYL )

=> s l10 not l11

L12 36 L10 NOT L11

=> s l12 and penty?

97437 PENTY?

L13 0 L12 AND PENTY?

=> d ide l12 30

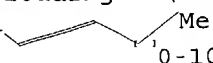
L12 ANSWER 30 OF 36 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	1851103
Beilstein Pref. RN (BPR):	60851-88-9
CAS Reg. No. (RN):	60851-88-9
Chemical Name (CN):	3-decyloxy-propan-1-ol
Autonom Name (AUN):	3-decyloxy-propan-1-ol
Molec. Formula (MF):	C13 H28 O2
Molecular Weight (MW):	216.36
Lawson Number (LN):	523, 362
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	1696104
Tautomer ID (TAUTID):	1757099
Beilstein Citation (BSO):	5-01, 6-01
Entry Date (DED):	1989/06/29
Update Date (DUPD):	2003/10/23

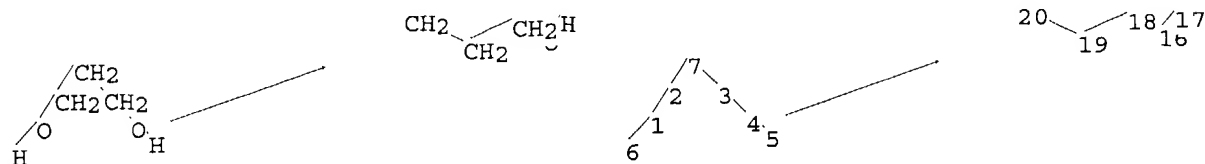


Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	2
ED	Entry Date	1

=>  
 Uploading C:\Program Files\Stnexp\Queries\10679174.str  
 G1  0-10

*Search*



chain nodes :  
 1 2 3 4 5 6 7 8 9 10 12 13 16 17 18 19 20  
 chain bonds :  
 1-2 1-6 2-7 3-4 3-7 4-5 8-9 8-10 9-12 12-13 16-17 16-18 18-19 19-20  
 exact/norm bonds :  
 8-10  
 exact bonds :  
 1-2 1-6 2-7 3-4 3-7 4-5 8-9 9-12 12-13 16-17 16-18 18-19 19-20

G1:H,Ak,Cb

Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
 10:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
 fragments assigned product role:  
 containing 16  
 fragments assigned reactant/reagent role:  
 containing 1  
 containing 8

L1 STRUCTURE UPLOADED

=> d  
 L1 HAS NO ANSWERS  
 L1 STR  
 \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
 SAMPLE SEARCH INITIATED 13:47:04 FILE 'CASREACT'  
 SCREENING COMPLETE - 4638 REACTIONS TO VERIFY FROM 446 DOCUMENTS

100.0% DONE 4638 VERIFIED 0 HIT RXNS 0 DOCS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 88699 TO 96821  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 13:47:11 FILE 'CASREACT'

SCREENING COMPLETE - 98286 REACTIONS TO VERIFY FROM 9143 DOCUMENTS

100.0% DONE 98286 VERIFIED 11 HIT RXNS 6 DOCS  
SEARCH TIME: 00.00.12

L3 6 SEA SSS FUL L1 ( 11 REACTIONS)

=> d ibib abs fhit 1-6

L3 ANSWER 1 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 135:14317 CASREACT

TITLE: Nervonic acid derivatives, their preparation, and  
anti-inflammatory and immunomodulatory use

INVENTOR(S): Coupland, Keith; Raoul, Yann

PATENT ASSIGNEE(S): Croda International PLC, UK

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

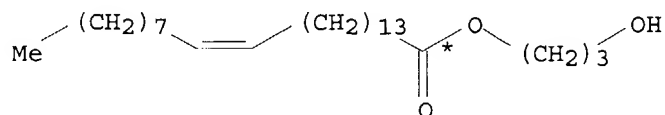
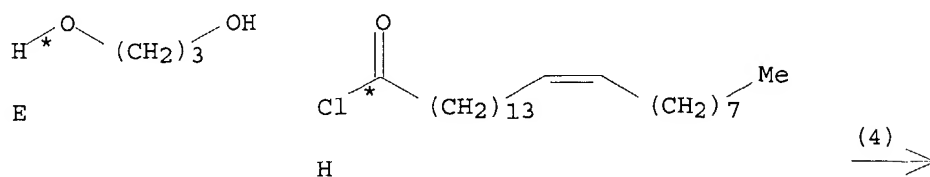
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001038288	A1	20010531	WO 2000-GB4453	20001123
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,				
HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,				
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,				
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,				
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,				
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
GB 2357083	A1	20010613	GB 2000-28525	20001123
GB 2357083	B2	20020619		
EP 1232139	A1	20020821	EP 2000-977695	20001123
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003514886	T2	20030422	JP 2001-539845	20001123
NZ 518961	A	20040227	NZ 2000-518961	20001123
US 6664406	B1	20031216	US 2002-130672	20020819
PRIORITY APPLN. INFO.:			GB 1999-27629	19991124
			WO 2000-GB4453	20001123

OTHER SOURCE(S): MARPAT 135:14317

AB The invention discloses nervonic acid derivs.

CH<sub>3</sub>(CH<sub>2</sub>)<sub>7</sub>CH:CH(CH<sub>2</sub>)<sub>13</sub>C(O)O(CH<sub>2</sub>)<sub>3</sub>OR (R = H, carboxylic acid residue), or a salt of the compound where R is H, or a bioprecursor, prodrug or hydrate thereof. Those compds. wherein R is other than H have pharmacol. activity, in particular anti-inflammatory and immunomodulatory effects. Those compds. wherein R is H can be used to prepare the pharmacol. active derivs.

RX(4) OF 14 ...E + H ==> A...



A

RX(4) RCT E 504-63-2

STAGE(1)

RGT K 121-44-8 Et3N

SOL 75-09-2 CH2Cl2

STAGE(2)

RCT H 145411-43-4

SOL 75-09-2 CH2Cl2

PRO A 342573-48-2

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 114:42757 CASREACT

TITLE: Synthesis of methyl-substituted lariat ethers containing a 13-crown-4 ring

AUTHOR(S): Wakita, Ryuhei; Yonetani, Masayuki; Nakatsuji, Yohji; Okahara, Mitsuo

CORPORATE SOURCE: Fac. Eng., Osaka Univ., Osaka, 565, Japan

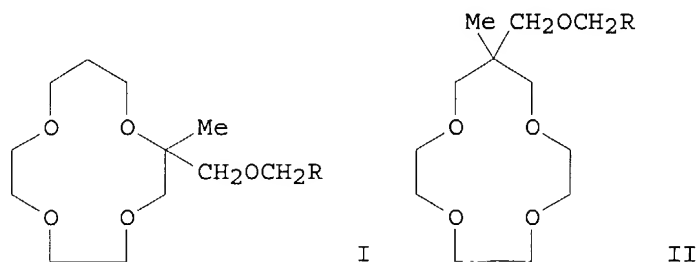
SOURCE: Journal of Heterocyclic Chemistry (1990), 27(5), 1337-9

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

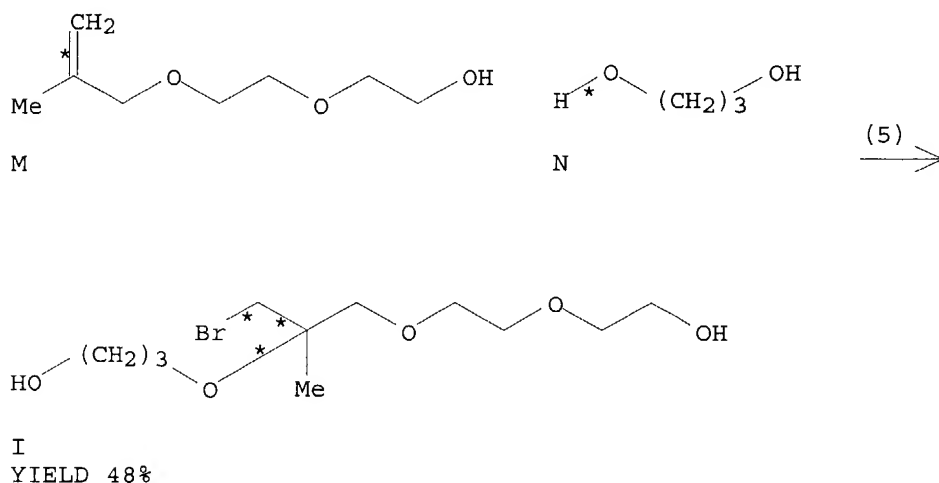
GI



AB Convenient synthetic procedures for preparing two kinds of methyl-substituted

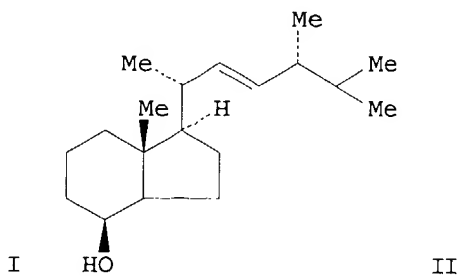
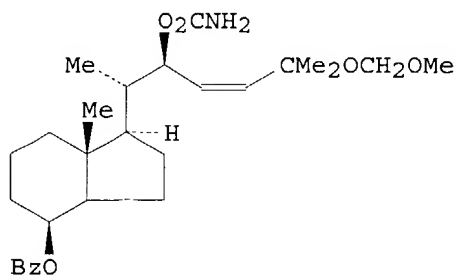
lariat ethers containing a 13-crown-4-ring, I and II [R = CH<sub>2</sub>OMe, (CH<sub>2</sub>)<sub>8</sub>Me, 2-tetrahydrofuryl], are described. I were obtained from the reaction of 2-bromomethyl-2-methyl-13-crown-4 (III) with the appropriate alkoxide. III was prepared without the need for prior protection of the bromomethyl group. For the synthesis of II, which possess an electron-donating group on the central carbon of the tri-Me moiety of the 13-crown-4-ring, the substituents were introduced before cyclization.

RX(5) OF 9      M + N ==> I...



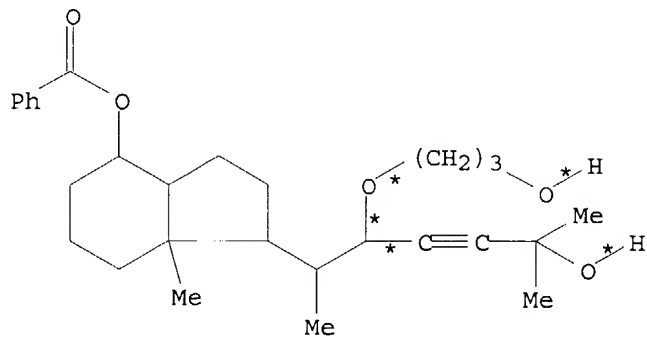
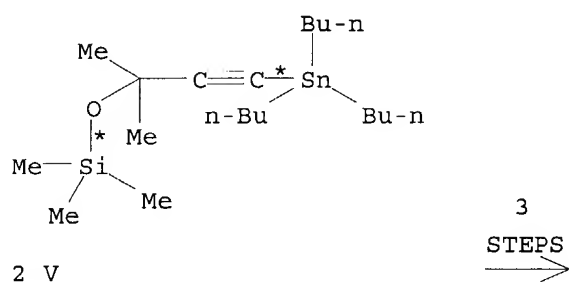
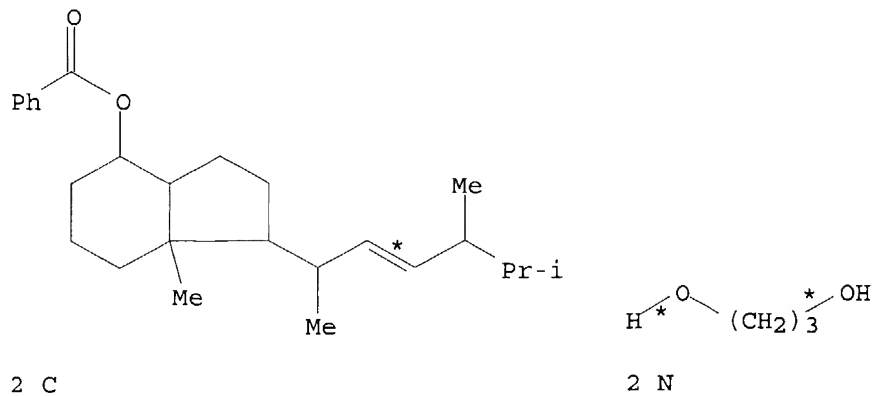
RX(5)      RCT    M 121343-32-6, N 504-63-2  
              RGT    L 128-08-5 Bromosuccinimide  
              PRO    I 131526-53-9  
              SOL    504-63-2 HO(CH<sub>2</sub>)<sub>3</sub>OH

L3    ANSWER 3 OF 6    CASREACT    COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER:      109:73744    CASREACT  
 TITLE:                    Stereoselective synthesis of 25-hydroxyvitamin D<sub>2</sub> side chain via the acetal template route  
 AUTHOR(S):               Castedo, L.; Granja, J.; Maestro, M. A.; Mourino, A.  
 CORPORATE SOURCE:      Dep. Quim. Org., Fac. Quim., Santiago de Compostela, Spain  
 SOURCE:                   Tetrahedron Letters (1987), 28(39), 4589-90  
                              CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE:          Journal  
 LANGUAGE:                English  
 GI

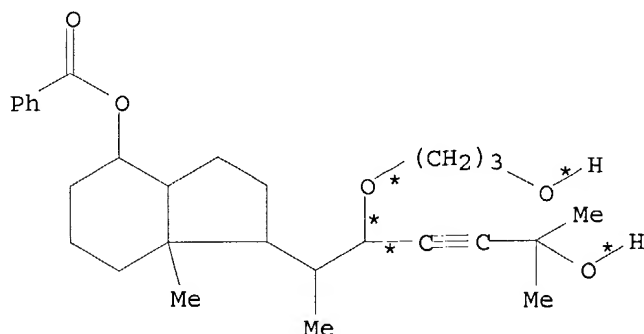


AB An improved synthesis of the vitamin intermediate I from II was described.

RX(31) OF 54 COMPOSED OF RX(2), RX(4), RX(8)  
 RX(31) 2 C + 2 N + 2 V ==> W + X



YIELD 85%(67)



X  
YIELD 85% (33)

RX(2) RCT C 68702-86-3

STAGE(1)

RGT G 10028-15-6 Ozone, D 110-86-1 Pyridine  
SOL 67-56-1 MeOH, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT H 122-52-1 P(OEt)<sub>3</sub>  
SOL 67-56-1 MeOH, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
PRO F 66774-71-8

RX(4) RCT N 504-63-2, F 66774-71-8  
RGT P 109-63-7 BF<sub>3</sub>-Et<sub>2</sub>O  
PRO O 115527-13-4  
SOL 109-99-9 THF

RX(8) RCT V 115527-16-7, O 115527-13-4  
RGT Y 7550-45-0 TiCl<sub>4</sub>  
PRO W 115527-17-8, X 115589-94-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

L3 ANSWER 4 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 107:133679 CASREACT

TITLE: Thermal reactions of cyclopropenone ketals. Key mechanistic features and scope of the cycloaddition reactions of delocalized singlet vinylcarbenes: three-carbon 1,1-/1,3-dipoles

AUTHOR(S): Boger, Dale L.; Brotherton, Christine E.

CORPORATE SOURCE: Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045-2500, USA

SOURCE: Journal of the American Chemical Society (1986), 108(21), 6695-713

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

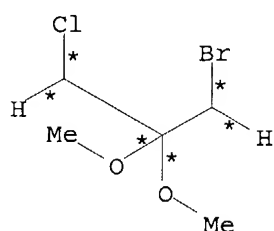
LANGUAGE: English

AB Full details of the key mechanistic features and the preparative scope of the thermal reactions of cyclopropenone ketals which proceed by the thermal generation and subsequent cycloaddn. reactions of  $\pi$ -delocalized singlet vinylcarbenes, 3-carbon 1,1-/1,3-dipoles lacking octet stabilization, are described and include  $\omega$ 2a participation in cheletropic [ $\pi$ 2s +  $\omega$ 2a] nonlinear cycloaddns. with an observable endo effect suitable for a one-step, stereoselective construction of cis-cyclopropaneacetic acid esters, formal  $\pi$ 2a participation in [ $\pi$ 2s +  $\pi$ 2a] cycloaddns. suitable for the preparation of functionalized

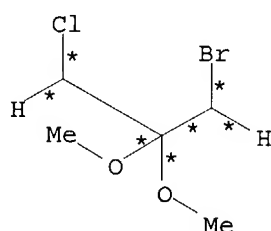


cyclopentenones in which each of the 5 carbons of the newly formed 5-membered ring may bear functionality capable of addnl. transformation, and  $\pi 2a$  participation in  $[\pi 4s + \pi 2s]$  cycloaddns. with selected dienes in direct  $[3 + 4]$  cycloaddns. suitable for the preparation of functionalized cycloheptadienes capable of further elaboration to tropones/tropolones. The complementary scope of the thermal reactions of cyclopropenone ketals is demonstrated with the preparation of the complete range of (methoxycarbonyl)tropones, 2-, 3-, and 4-(methoxycarbonyl)tropone and tropone, utilizing the appropriate choice of starting diene and complementary choice of conditions for promoting the thermal  $[3 + 4]$  or  $[4 + 2]$  cycloaddn. of a cyclopropenone ketal. Addnl. details of a preliminary study of the scope of the cycloaddn. reactions of the apparent  $\pi$ -delocalized singlet vinylcarbene with C-heteroatom double bonds are described.

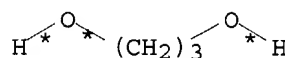
RX(91) OF 123 COMPOSED OF RX(51), RX(52), RX(6)  
 RX(91) 2 CO + 2 CP + 2 N ==> O + M



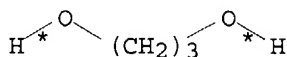
CO



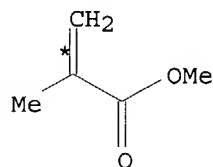
CO



CP

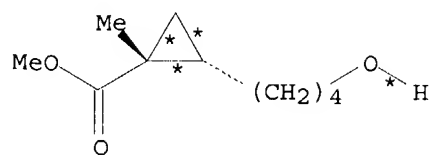


CP

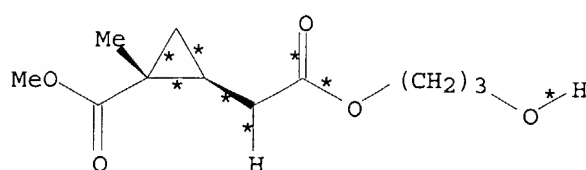


2 N

3  
STEPS  
→



O



M

RX(51) RCT CO 22089-54-9, CP 504-63-2  
 RGT CM 7664-93-9 H2SO4  
 PRO CQ 60935-30-0  
 SOL 7732-18-5 Water

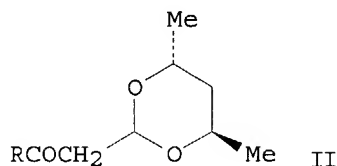
RX(52) RCT CQ 60935-30-0

RGT CR 17242-52-3 KNH2  
 PRO A 60935-21-9  
 CAT 7705-08-0 FeCl3  
 SOL 7664-41-7 NH3, 60-29-7 Et2O

RX(6) RCT A 60935-21-9, N 80-62-6  
 PRO O 103384-75-4, M 94923-06-5  
 SOL 71-43-2 Benzene

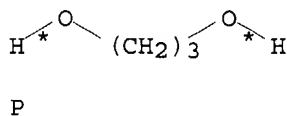
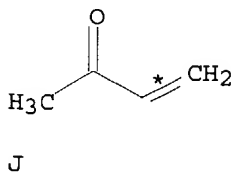
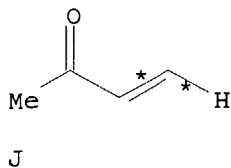
L3 ANSWER 5 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

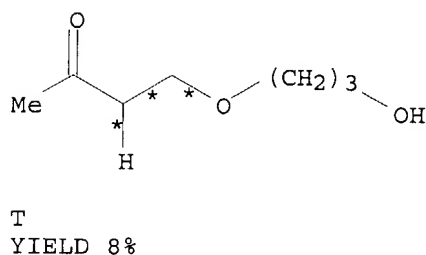
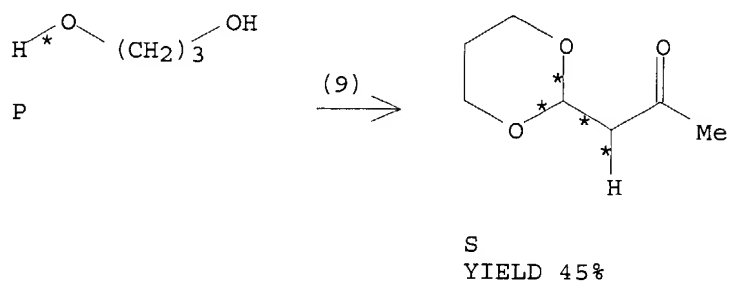
ACCESSION NUMBER: 106:213861 CASREACT  
 TITLE: Palladium(II)-catalyzed acetalization of terminal  
 olefins bearing electron-withdrawing substituents with  
 optically active diols  
 AUTHOR(S): Hosokawa, Takahiro; Ohta, Toshiyuki; Kanayama,  
 Satoshi; Murahashi, Shunichi  
 CORPORATE SOURCE: Fac. Eng. Sci., Osaka Univ., Osaka, 560, Japan  
 SOURCE: Journal of Organic Chemistry (1987), 52(9), 1758-64  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Terminal alkenes bearing electron-withdrawing substituents, such as  $\text{CH}_2\text{:CH}_2\text{:CHCOR}$  ( $\text{R} = \text{Ph}, \text{Me}, \text{Me}_3\text{C}$ ),  $\text{CH}_2\text{:CHCO}_2\text{Me}$ , and  $\text{CH}_2\text{:CHCN}$ , are regioselectively acetalized at the terminal carbon by diols in the presence of  $\text{PdCl}_2$  and  $\text{CuCl}$  in  $\text{MeOCH}_2\text{CH}_2\text{OMe}$  at  $50^\circ$  under an atmospheric of  $\text{O}$ . The use of optically active ( $R,R$ )-2,4-pentanediol (I) gives homochiral cyclic acetals of aldehyde precursors, for example, II ( $\text{R} = \text{Ph}, \text{Me}, \text{Me}_3\text{C}$ ), in good yields. The reactivity of alkenes appears to decrease in the order:  $\text{CH}_2\text{:CHPh} > \text{CH}_2\text{:CHCO}_2\text{Me} > \text{CH}_2\text{:CHCOR}$ . Acetalization of  $\text{CH}_2\text{:CHCOR}$  is accompanied by the formation of Michael-type adducts such as  $\text{RCOCH}_2\text{CH}_2\text{OCHMeCH}_2\text{CH(OH)Me}$ . Their formation can be prevented by the use of  $\text{Na}_2\text{HPO}_4$  as an additive. Although in an early stage of the reaction of  $\text{CD}_2\text{:CHPh}$  with I, a statistical D scrambling of the starting alkene occurs, no such scrambling is observed with  $\text{CD}_2\text{:CHCOPh}$ . Addnl., the acetalization of  $\text{CD}_2\text{:CHCOPh}$  with I results in 1,2 deuterium migration, together with 25% D loss. These results are explained by reaction pathways involving oxypalladation, Pd-H elimination, and subsequent ring closure giving enol ether. A catalytic cycle involving the oxygenation of Pd-H species with mol. oxygen is proposed.

RX(9) OF 36 2 J + 2 P ==> S + T...

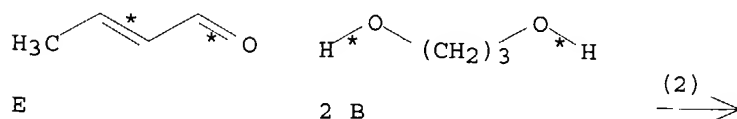


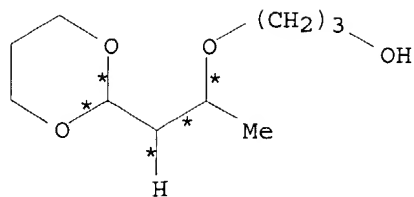


RX(9)      RCT   J 78-94-4, P 504-63-2  
             RGT   E 7782-44-7 O2  
             PRO   S 55558-31-1, T 87971-38-8  
             CAT   7647-10-1 PdCl2, 7758-89-6 CuCl  
             SOL   110-71-4 (CH2OMe)2

L3    ANSWER 6 OF 6    CASREACT    COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER:      102:220779    CASREACT  
 TITLE:                    Acetals and ethers - XIII. Reaction products of  
                               2-butenal with ethylene glycol  
 AUTHOR(S):                Piasecki, Andrzej  
 CORPORATE SOURCE:        Inst. Org. Polym. Technol., Techn. Univ. Wroclaw,  
                               Wroclaw, 50-370, Pol.  
 SOURCE:                    Tetrahedron (1984), 40(23), 4893-6  
                               CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE:            Journal  
 LANGUAGE:                 English  
 AB    The unsatd. cyclic acetal, 2-(1-propenyl)-1,3-dioxolane, was an  
       intermediate in the 4-MeC6H4SO3H-catalyzed reaction of 2-butenal with  
       excess ethylene glycol. The final product was 2-[2-(2-  
       hydroxyethoxy)propyl]-1,3-dioxolane, and a small amount of cis- and  
       trans-5-(2-hydroxyethoxy)-7-methyl-1,4-dioxepane.

RX(2) OF 8      E + 2 B ==> F





F

RX(2) RCT E 4170-30-3, B 504-63-2  
 PRO F 96424-48-5  
 CAT 104-15-4 TSOH

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
130.20	131.37

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-3.96	-3.96

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STRUCTURE FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7  
 DICTIONARY FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> s tsoh

L4 0 TSOH  
 0 TSOH

=> s 104-15-4

L5 1 104-15-4  
 (104-15-4/RN)

=> d

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 104-15-4 REGISTRY  
 CN Benzenesulfonic acid, 4-methyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN p-Toluenesulfonic acid (7CI, 8CI)

OTHER NAMES:

CN 4-Methylbenzenesulfonic acid

CN 4-Toluenesulfonic acid

CN Cyzac 4040

CN K-Cure 1040

CN Nacure 1040

CN NSC 167068

CN NSC 2167

CN p-Methylbenzenesulfonic acid

CN p-Methylphenylsulfonic acid

CN p-Toluenesulphonic acid

CN p-Tolylsulfonic acid

CN PTS 100

CN Toluenesulfonic acid

CN Tosic acid

AR 25231-46-3, 633305-48-3

FS 3D CONCORD

DR 402-47-1, 128739-80-0, 126033-27-0, 114213-96-6, 156627-46-2, 144647-92-7,  
100901-72-2, 210357-81-6, 227313-49-7, 369371-25-5, 613262-31-0

MF C7 H8 O3 S

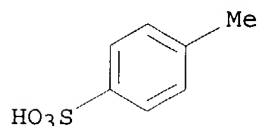
CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,  
CHEMINFORMRX, CHEMLIST, CIN, CSCHM, CSNB, DETHERM\*, DIPPR\*, EMBASE,  
ENCOMPLIT, ENCOMPLIT2, ENCOMPAT, ENCOMPAT2, GMELIN\*, HODOC\*, HSDB\*,  
IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK\*, MSDS-OHS, NIOSHTIC,  
PDLCOM\*, PIRA, PROMT, PS, RTECS\*, SPECINFO, TOXCENTER, TULSA, ULIDAT,  
USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9631 REFERENCES IN FILE CA (1907 TO DATE)

356 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

9644 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d it 6 l3

YOU HAVE REQUESTED DATA FROM FILE 'CASREACT' - CONTINUE? (Y)/N:y

L3 ANSWER 6 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

IT Acetals

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclic, of butenal)

IT 96424-45-2P 96424-46-3P 96424-50-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and methylation or transacetalization of)

IT 96424-44-1P 96424-47-4P 96424-48-5P 96424-49-6P 96424-51-0P  
96424-52-1P 96424-53-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

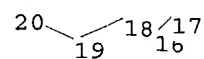
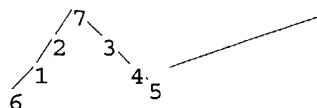
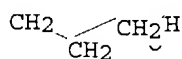
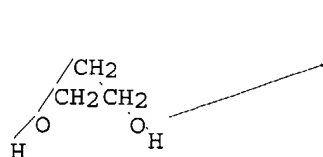
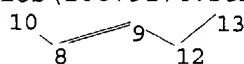
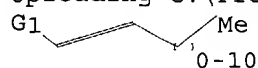
IT 123-73-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with ethylene glycol or ethylene glycol monomethyl ether  
and trimethylene glycol)

=>

Uploading C:\Program Files\Stnexp\Queries\10679174.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 12 13 16 17 18 19 20

chain bonds :

1-2 1-6 2-7 3-4 3-7 4-5 8-9 8-10 9-12 12-13 16-17 16-18 18-19 19-20

exact/norm bonds :

8-10

exact bonds :

1-2 1-6 2-7 3-4 3-7 4-5 8-9 9-12 12-13 16-17 16-18 18-19 19-20

G1:H,Ak,Cb

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS

fragments assigned product role:

containing 16

fragments assigned reactant/reagent role:

containing 1

containing 8

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:22:07 FILE 'CASREACT'

SCREENING COMPLETE - 10610 REACTIONS TO VERIFY FROM 687 DOCUMENTS

47.1% DONE 5000 VERIFIED 0 HIT RXNS

0 DOCS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 206105 TO 218295  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 15:22:12 FILE 'CASREACT'

SCREENING COMPLETE - 202587 REACTIONS TO VERIFY FROM 13630 DOCUMENTS

100.0% DONE 202587 VERIFIED 24 HIT RXNS 10 DOCS  
SEARCH TIME: 00.00.17

L3 10 SEA SSS FUL L1 ( 24 REACTIONS)

=> d his

(FILE 'HOME' ENTERED AT 15:21:00 ON 15 APR 2004)

FILE 'REGISTRY' ENTERED AT 15:21:15 ON 15 APR 2004

FILE 'CASREACT' ENTERED AT 15:21:27 ON 15 APR 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 10 S L1 FULL

=> d ibib abs fhit 1-10

L3 ANSWER 1 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 135:14317 CASREACT

TITLE: Nervonic acid derivatives, their preparation, and  
anti-inflammatory and immunomodulatory use

INVENTOR(S): Coupland, Keith; Raoul, Yann

PATENT ASSIGNEE(S): Croda International PLC, UK

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001038288	A1	20010531	WO 2000-GB4453	20001123
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW:				
GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
GB 2357083	A1	20010613	GB 2000-28525	20001123
GB 2357083	B2	20020619		
EP 1232139	A1	20020821	EP 2000-977695	20001123
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003514886	T2	20030422	JP 2001-539845	20001123
NZ 518961	A	20040227	NZ 2000-518961	20001123
US 6664406	B1	20031216	US 2002-130672	20020819
PRIORITY APPLN. INFO.:			GB 1999-27629	19991124
			WO 2000-GB4453	20001123

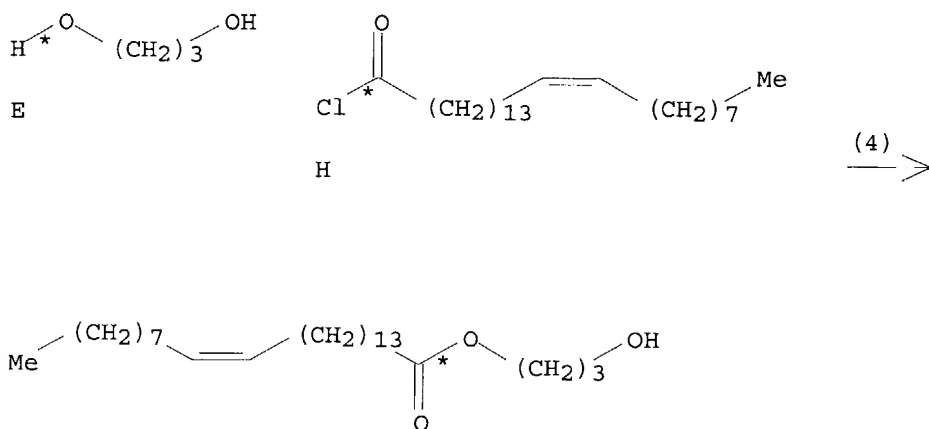


OTHER SOURCE(S): MARPAT 135:14317

AB The invention discloses nervonic acid derivs.

CH<sub>3</sub>(CH<sub>2</sub>)<sub>7</sub>CH:CH(CH<sub>2</sub>)<sub>13</sub>C(O)O(CH<sub>2</sub>)<sub>3</sub>OR (R = H, carboxylic acid residue), or a salt of the compound where R is H, or a bioprecursor, prodrug or hydrate thereof. Those compds. wherein R is other than H have pharmacol. activity, in particular anti-inflammatory and immunomodulatory effects. Those compds. wherein R is H can be used to prepare the pharmacol. active derivs.

RX(4) OF 14 ...E + H ==> A...



A

RX(4) RCT E 504-63-2

STAGE(1)

RGT K 121-44-8 Et3N

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RCT H 145411-43-4

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

PRO A 342573-48-2

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 128:102040 CASREACT

TITLE: Functionalized ozonides by substitution reactions of chlorinated ozonides with difunctional alcohols

AUTHOR(S): Griesbaum, Karl; Quinkert, Ralf Olaf

CORPORATE SOURCE: Engler-Bunte-Institut, Bereich Petrochemie, Universitaet Karlsruhe, Karlsruhe, D-76128, Germany

SOURCE: Liebigs Annalen/Recueil (1997), (12), 2581-2585

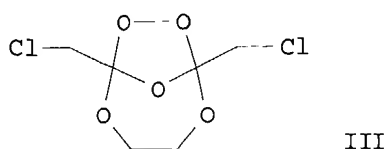
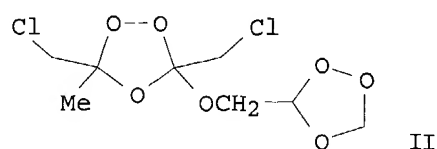
CODEN: LIARFV

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

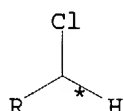
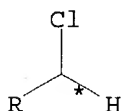
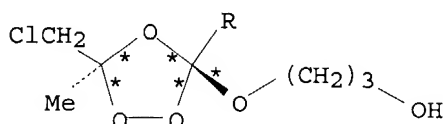
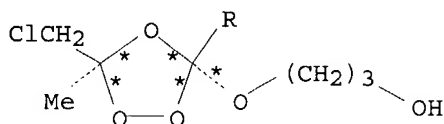
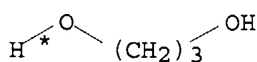
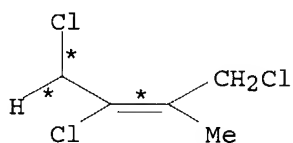
LANGUAGE: English

GI



AB Substitution of 3-chloro-3,5-bis(chloromethyl)-5-methyl-1,2,4-trioxolane (I) with allyl alc. gave the corresponding diastereomeric allyloxy-substituted ozonides, which were converted into diozonides II by ozone treatment. Substitution of I with ethanediol or with 1,3-propanediol gave the corresponding hydroxyalkoxy-substituted ozonides, which were oxidized to the corresponding aldehydes. Reaction of 3,5-dichloro-3,5-bis(chloromethyl)-1,2,4-trioxolane with ethanediol gave the corresponding bis(hydroxy)-substituted ozonide as well as bicyclic ozonide III by reaction with ethanediol in a ratio of 1:1.

RX(10) OF 19      2 A + 2 Z ==> AA + X...



AA  
YIELD 12%

X  
YIELD 35%

RX(10)      RCT   A 73900-41-1

STAGE(1)

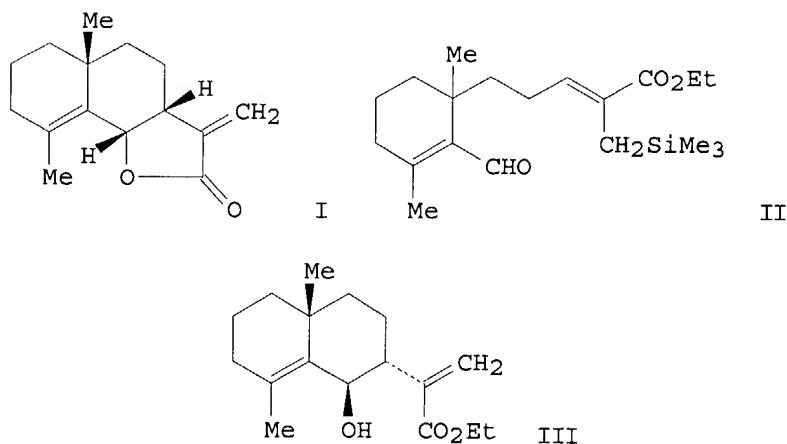
RGT   E 10028-15-6 Ozone  
SOL   109-66-0 Pentane

STAGE(2)

RCT   Z 504-63-2  
RGT   F 584-08-7 K2CO3

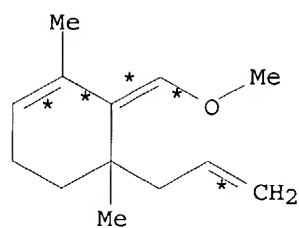
STAGE(3)

L3 ANSWER 3 OF 10 CASREACT COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 120:107377 CASREACT  
TITLE: Synthesis of a stereoisomer of frullanolide utilizing  
the intramolecular cyclization of  $\omega$ -formyl-2-  
alkenylsilane  
AUTHOR(S): Kuroda, Chiaki; Shimizu, Shigeru; Haishima, Takahiro;  
Sato, James Y.  
CORPORATE SOURCE: Dep. Chem., Rikkyo Univ., Tokyo, 171, Japan  
SOURCE: Bulletin of the Chemical Society of Japan (1993),  
66(8), 2298-303  
CODEN: BCSJA8; ISSN: 0009-2673  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

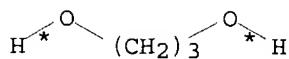


AB Synthesis of 10-epi-frullanolide (I) is reported via the intramol. cyclization of a  $\omega$ -formyl- $\alpha$ -trimethylsilylmethyl- $\alpha,\beta$ -unsatd. ester. The cyclization precursor, Et (Z)-5-(2-formyl-1,3-dimethyl-2-cyclohexenyl)-2-trimethylsilylmethyl-2-pentenoate (II), was prepared from 2,6-dimethyl-2-cyclohexen-1-one through the dialdehyde monoacetal as the key intermediate. Cyclization of II with tetrabutylammonium fluoride produced the hydroxy ester III having C(6 $\alpha$ )-H and C(7 $\beta$ )-H, which was hydrolyzed, then subjected to Fujisawa's lactonization to afford I.

RX(13) OF 55 COMPOSED OF RX(4), RX(5)  
RX(13) Q + S ==> Y

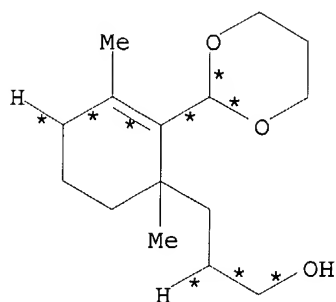


Q



S

2  
STEPS  
→



Y

YIELD 96%

RX(4) RCT Q 152429-50-0

STAGE(1)

RGT U 7647-01-0 HCl

SOL 7732-18-5 Water, 109-99-9 THF

STAGE(2)

RCT S 504-63-2

CAT 24057-28-1 Pyridinium tosylate

SOL 71-43-2 Benzene

PRO T 152429-52-2

RX(5) RCT T 152429-52-2

STAGE(1)

RGT Z 109-63-7 BF3-Et2O, AA 16940-66-2 NaBH4, AB

513-35-9 Me2C:CHMe

SOL 513-35-9 Me2C:CHMe

STAGE(2)

RGT AC 7722-84-1 H2O2, AD 1310-73-2 NaOH

SOL 7732-18-5 Water

PRO Y 152429-54-4

L3 ANSWER 4 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 115:280316 CASREACT

TITLE: Synthesis of (+)-fragolide and (-)-pereniporin B via vinylsilane terminated cationic cyclization

AUTHOR(S): Burke, Steven D.; Shankaran, K.; Helber, Margaret Jones

CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

GI

Dep. Chem., Univ. Wisconsin, Madison, WI, 53706, USA

Tetrahedron Letters (1991), 32(36), 4655-8

CODEN: TELEAY; ISSN: 0040-4039

Journal

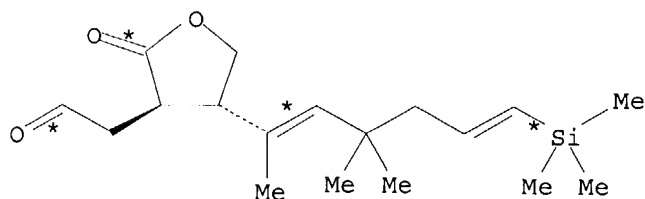
English

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

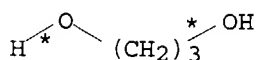
AB Enantioselective syntheses of (+)-fragolide (I) and (-)-pereniporin B (II) are detailed. Marino's lactone annulation method, reaction of sulfone III and ZnCu/Cl<sub>3</sub>COCl to give lactone IV, was employed to establish relative and absolute stereochem. at carbon in the bicyclization substrate. Regio- and stereoselective oxidns. of tricyclic drimane precursors are described.

RX(35) OF 119 COMPOSED OF RX(5), RX(6), RX(7)

RX(35) 2 P + 2 Q ==> V + W

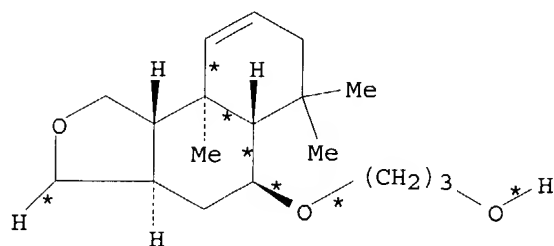


2 P

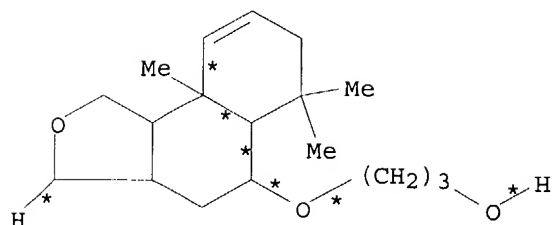


2 Q

3  
STEPS  
→



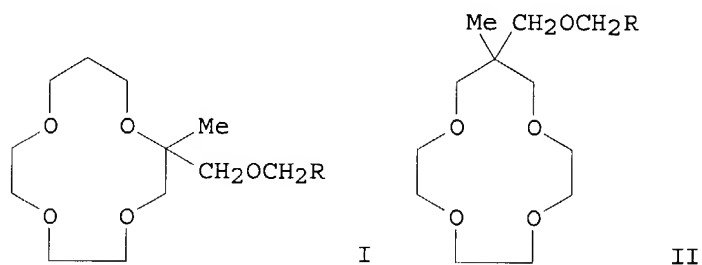
V



W

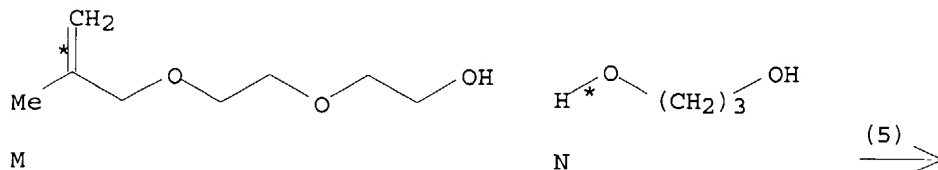
RX(5) RCT P 137266-31-0, Q 504-63-2  
 RGT S 77-78-1 Me<sub>2</sub>SO<sub>4</sub>  
 PRO R 137266-24-1  
 SOL 68-12-2 DMF  
 NTE 4Å zeolites  
  
 RX(6) RCT R 137266-24-1  
 PRO U 137266-25-2  
 NTE 2 steps  
  
 RX(7) RCT U 137266-25-2  
 RGT X 7550-45-0 TiCl<sub>4</sub>  
 PRO V 137266-26-3, W 137331-24-9  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 NTE key step; 85% overall

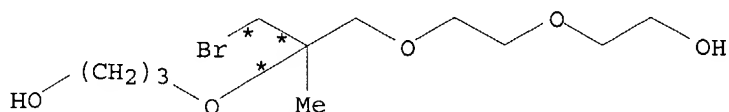
L3 ANSWER 5 OF 10 CASREACT COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 114:42757 CASREACT  
 TITLE: Synthesis of methyl-substituted lariat ethers  
 containing a 13-crown-4 ring  
 AUTHOR(S): Wakita, Ryuhei; Yonetani, Masayuki; Nakatsuji, Yohji;  
 Okahara, Mitsuo  
 CORPORATE SOURCE: Fac. Eng., Osaka Univ., Osaka, 565, Japan  
 SOURCE: Journal of Heterocyclic Chemistry (1990), 27(5),  
 1337-9  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Convenient synthetic procedures for preparing two kinds of methyl-substituted lariat ethers containing a 13-crown-4-ring, I and II [R = CH<sub>2</sub>OMe, (CH<sub>2</sub>)<sub>8</sub>Me, 2-tetrahydrofuryl], are described. I were obtained from the reaction of 2-bromomethyl-2-methyl-13-crown-4 (III) with the appropriate alkoxide. III was prepared without the need for prior protection of the bromomethyl group. For the synthesis of II, which possess an electron-donating group on the central carbon of the tri-Me moiety of the 13-crown-4-ring, the substituents were introduced before cyclization.

RX(5) OF 9      M + N ==> I...





I

YIELD 48%

RX(5) RCT M 121343-32-6, N 504-63-2  
 RGT L 128-08-5 Bromosuccinimide  
 PRO I 131526-53-9  
 SOL 504-63-2 HO(CH<sub>2</sub>)<sub>3</sub>OH

L3 ANSWER 6 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 113:40247 CASREACT

TITLE: Synthesis of optically active mevinic acid subunits  
 via acetal initiated/vinylsilane terminated polyene  
 cyclizations

AUTHOR(S): Burke, Steven D.; Takeuchi, Kumiko; Murtiashaw, C. W.;  
 Liang, D. W. M.

CORPORATE SOURCE: Dep. Chem., Univ. South Carolina, Columbia, SC, 29208,  
 USA

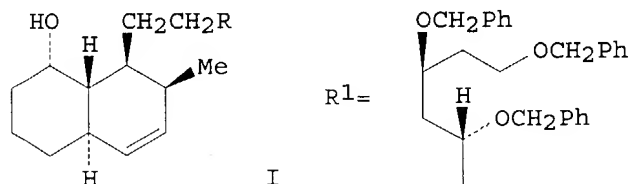
SOURCE: Tetrahedron Letters (1989), 30(46), 6299-302

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

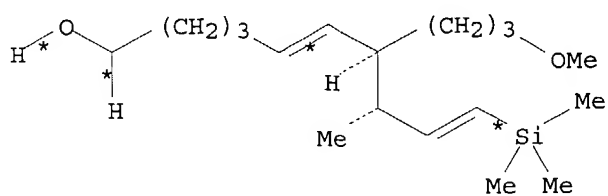
GI



AB Efficient routes to optically active octahydronaphthalenol mevinic acid  
 subunits I (R = CH<sub>2</sub>OMe, R1) via vinylsilane-mediated polyene cyclizations  
 initiated by trimethylenedioxy acetals are detailed. Enantioselective  
 alkynone redns. and Ireland-Claisen rearrangements serve to establish and  
 transfer absolute stereochem.

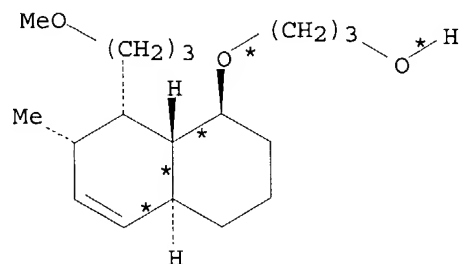
RX(26) OF 100 COMPOSED OF RX(7), RX(8)

RX(26) 3 AD ==> AL + AM + AN

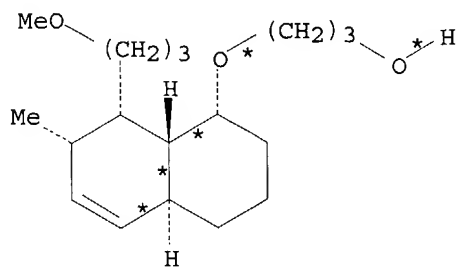


3 AD

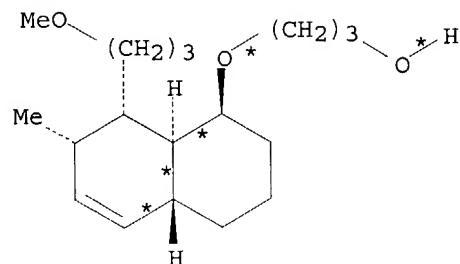
2  
STEPS  
→



AL  
YIELD 91% (17)



AM  
YIELD 91% (10)



AN  
YIELD 91% (73)

RX(7) RCT AD 128061-45-0

STAGE(1)

RGT W 79-37-8 (COCl)<sub>2</sub>, X 67-68-5 DMSO  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT Y 121-44-8 Et<sub>3</sub>N

STAGE(3)

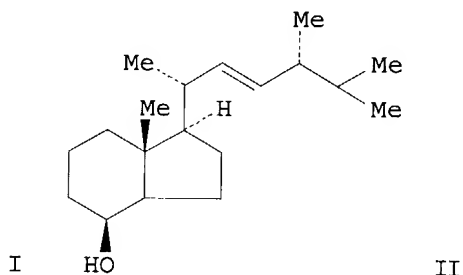
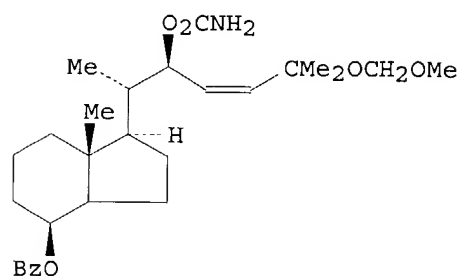
RGT AI 504-63-2 HO(CH<sub>2</sub>)<sub>3</sub>OH  
CAT 24057-28-1 Pyridinium tosylate  
SOL 71-43-2 Benzene  
PRO AH 128061-46-1

RX(8) RCT AH 128061-46-1



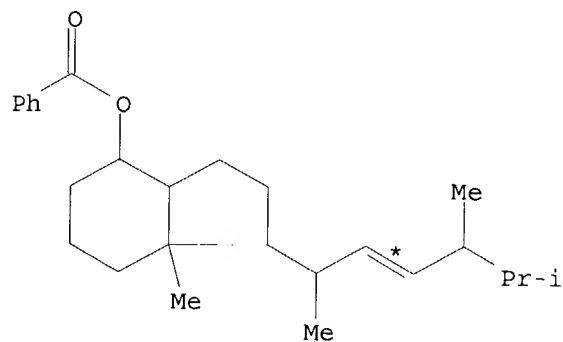
RGT AO 7550-45-0 TiCl4  
PRO AL 128038-02-8, AM 128038-03-9, AN 128038-04-0  
SOL 75-09-2 CH2Cl2

L3 ANSWER 7 OF 10 CASREACT COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 109:73744 CASREACT  
TITLE: Stereoselective synthesis of 25-hydroxyvitamin D2 side chain via the acetal template route  
AUTHOR(S): Castedo, L.; Granja, J.; Maestro, M. A.; Mourino, A.  
CORPORATE SOURCE: Dep. Quim. Org., Fac. Quim., Santiago de Compostela, Spain  
SOURCE: Tetrahedron Letters (1987), 28(39), 4589-90  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

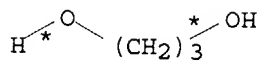


AB An improved synthesis of the vitamin intermediate I from II was described.

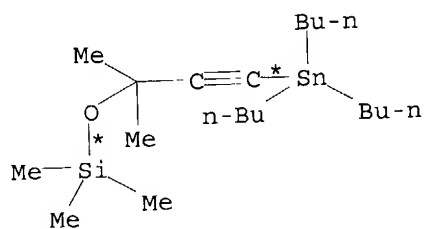
RX(31) OF 54 COMPOSED OF RX(2), RX(4), RX(8)  
RX(31) 2 C + 2 N + 2 V ==> W + X



2 C

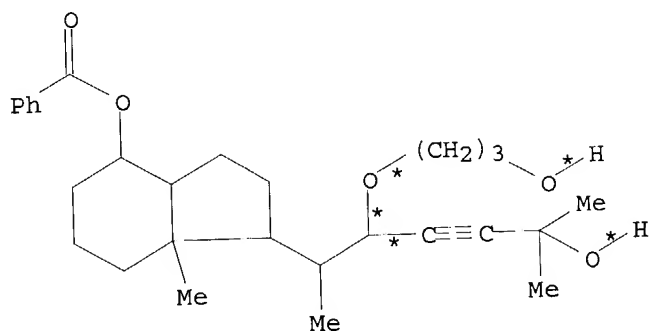


2 N

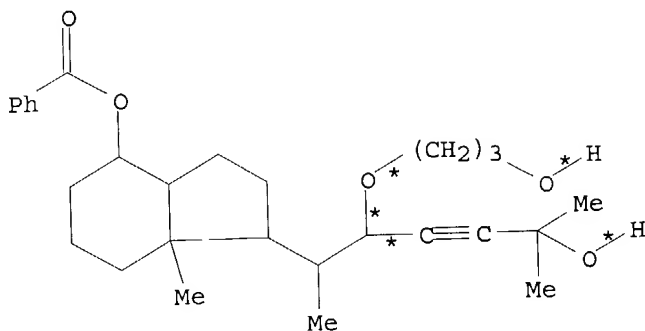


2 V

3  
STEPS  
→



W  
YIELD 85% (67)



X  
YIELD 85% (33)

RX(2) RCT C 68702-86-3

STAGE(1)

RGT G 10028-15-6 Ozone, D 110-86-1 Pyridine  
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2

STAGE(2)

RGT H 122-52-1 P(OEt)3  
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2  
PRO F 66774-71-8

RX(4) RCT N 504-63-2, F 66774-71-8  
 RGT P 109-63-7 BF3-Et2O  
 PRO O 115527-13-4  
 SOL 109-99-9 THF

RX(8) RCT V 115527-16-7, O 115527-13-4  
 RGT Y 7550-45-0 TiCl4  
 PRO W 115527-17-8, X 115589-94-1  
 SOL 75-09-2 CH2Cl2

L3 ANSWER 8 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 107:133679 CASREACT

TITLE: Thermal reactions of cyclopropenone ketals. Key mechanistic features and scope of the cycloaddition reactions of delocalized singlet vinylcarbenes: three-carbon 1,1-/1,3-dipoles

AUTHOR(S): Boger, Dale L.; Brotherton, Christine E.

CORPORATE SOURCE: Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045-2500, USA

SOURCE: Journal of the American Chemical Society (1986), 108(21), 6695-713

CODEN: JACSAT; ISSN: 0002-7863

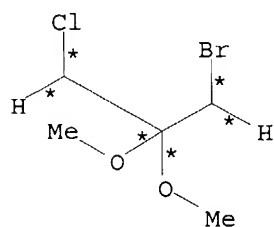
DOCUMENT TYPE: Journal

LANGUAGE: English

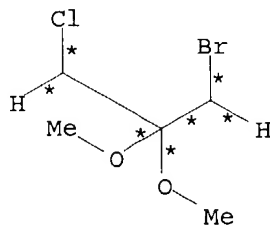
AB Full details of the key mechanistic features and the preparative scope of the thermal reactions of cyclopropenone ketals which proceed by the thermal generation and subsequent cycloaddn. reactions of  $\pi$ -delocalized singlet vinylcarbenes, 3-carbon 1,1-/1,3-dipoles lacking octet stabilization, are described and include  $\omega$ 2a participation in cheletropic [ $\pi$ 2s +  $\omega$ 2a] nonlinear cycloaddns. with an observable endo effect suitable for a one-step, stereoselective construction of cis-cyclopropaneacetic acid esters, formal  $\pi$ 2a participation in [ $\pi$ 2s +  $\pi$ 2a] cycloaddns. suitable for the preparation of functionalized cyclopentenenes in which each of the 5 carbons of the newly formed 5-membered ring may bear functionality capable of addnl. transformation, and  $\pi$ 2a participation in [ $\pi$ 4s +  $\pi$ 2s] cycloaddns. with selected dienes in direct [3 + 4] cycloaddns. suitable for the preparation of functionalized cycloheptadienes capable of further elaboration to tropones/tropolones. The complementary scope of the thermal reactions of cyclopropenone ketals is demonstrated with the preparation of the complete range of (methoxycarbonyl)tropones, 2-, 3-, and 4-(methoxycarbonyl)tropone and tropone, utilizing the appropriate choice of starting diene and complementary choice of conditions for promoting the thermal [3 + 4] or [4 + 2] cycloaddn. of a cyclopropenone ketal. Addnl. details of a preliminary study of the scope of the cycloaddn. reactions of the apparent  $\pi$ -delocalized singlet vinylcarbene with C-heteroatom double bonds are described.

RX(91) OF 123 COMPOSED OF RX(51), RX(52), RX(6)

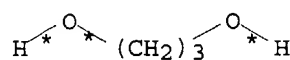
RX(91) 2 CO + 2 CP + 2 N ==> O + M



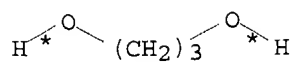
CO



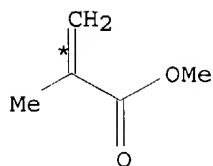
CO



CP

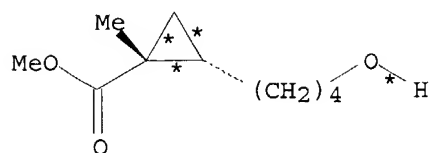


CP

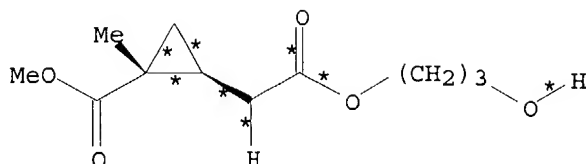


2 N

3  
STEPS  
→



O



M

RX(51) RCT CO 22089-54-9, CP 504-63-2  
RGT CM 7664-93-9 H2SO4  
PRO CQ 60935-30-0  
SOL 7732-18-5 Water

RX(52) RCT CQ 60935-30-0  
RGT CR 17242-52-3 KNH2  
PRO A 60935-21-9  
CAT 7705-08-0 FeCl3  
SOL 7664-41-7 NH3, 60-29-7 Et2O

RX(6) RCT A 60935-21-9, N 80-62-6  
PRO O 103384-75-4, M 94923-06-5  
SOL 71-43-2 Benzene

L3 ANSWER 9 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 106:213861 CASREACT

TITLE: Palladium(II)-catalyzed acetalization of terminal olefins bearing electron-withdrawing substituents with optically active diols

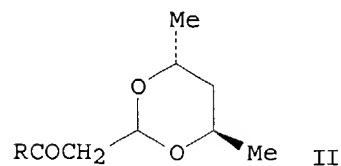
AUTHOR(S): Hosokawa, Takahiro; Ohta, Toshiyuki; Kanayama, Satoshi; Murahashi, Shunichi

CORPORATE SOURCE: Fac. Eng. Sci., Osaka Univ., Osaka, 560, Japan  
SOURCE: Journal of Organic Chemistry (1987), 52(9), 1758-64  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

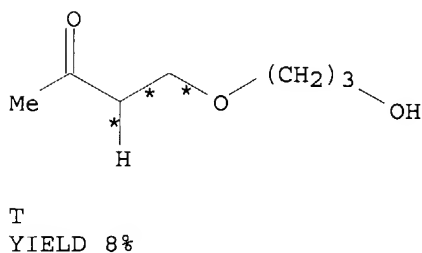
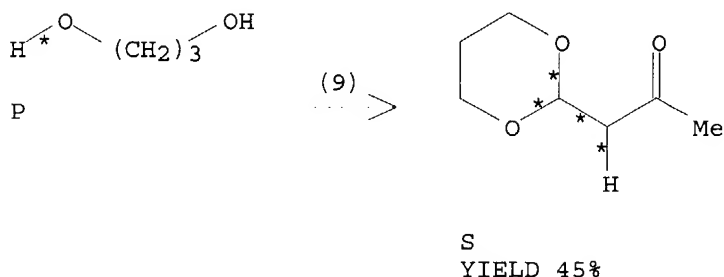
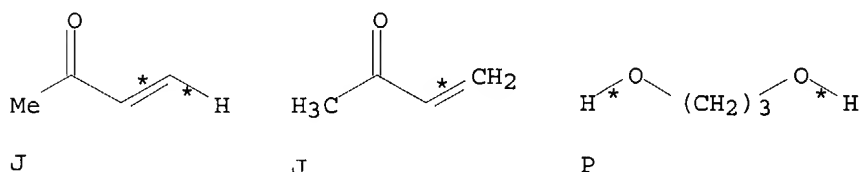
LANGUAGE: English

GI



AB Terminal alkenes bearing electron-withdrawing substituents, such as  $\text{CH}_2:\text{CH}_2:\text{CHCOR}$  ( $\text{R} = \text{Ph}, \text{Me}, \text{Me}_3\text{C}$ ),  $\text{CH}_2:\text{CHCO}_2\text{Me}$ , and  $\text{CH}_2:\text{CHCN}$ , are regioselectively acetalized at the terminal carbon by diols in the presence of  $\text{PdCl}_2$  and  $\text{CuCl}$  in  $\text{MeOCH}_2\text{CH}_2\text{OMe}$  at  $50^\circ$  under an atmospheric of  $\text{O}$ . The use of optically active (R,R)-2,4-pentanediol (I) gives homochiral cyclic acetals of aldehyde precursors, for example, II ( $\text{R} = \text{Ph}, \text{Me}, \text{Me}_3\text{C}$ ), in good yields. The reactivity of alkenes appears to decrease in the order:  $\text{CH}_2:\text{CHPh} > \text{CH}_2:\text{CHCO}_2\text{Me} > \text{CH}_2:\text{CHCOR}$ . Acetalization of  $\text{CH}_2:\text{CHCOR}$  is accompanied by the formation of Michael-type adducts such as  $\text{RCOCH}_2\text{CH}_2\text{OCHMeCH}_2\text{CH}(\text{OH})\text{Me}$ . Their formation can be prevented by the use of  $\text{Na}_2\text{HPO}_4$  as an additive. Although in an early stage of the reaction of  $\text{CD}_2:\text{CHPh}$  with I, a statistical D scrambling of the starting alkene occurs, no such scrambling is observed with  $\text{CD}_2:\text{CHCOPh}$ . Addnl., the acetalization of  $\text{CD}_2:\text{CHCOPh}$  with I results in 1,2 deuterium migration, together with 25% D loss. These results are explained by reaction pathways involving oxypalladation, Pd-H elimination, and subsequent ring closure giving enol ether. A catalytic cycle involving the oxygenation of Pd-H species with mol. oxygen is proposed.

RX(9) OF 36      2 J + 2 P ==> S + T...



RX(9)      RCT J 78-94-4, P 504-63-2  
 RGT E 7782-44-7 O2

PRO S 55558-31-1, T 87971-38-8  
CAT 7647-10-1 PdCl<sub>2</sub>, 7758-89-6 CuCl  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

L3 ANSWER 10 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 102:220779 CASREACT

TITLE: Acetals and ethers - XIII. Reaction products of  
2-butenal with ethylene glycol

AUTHOR(S): Piasecki, Andrzej

CORPORATE SOURCE: Inst. Org. Polym. Technol., Techn. Univ. Wroclaw,  
Wroclaw, 50-370, Pol.

SOURCE: Tetrahedron (1984), 40(23), 4893-6

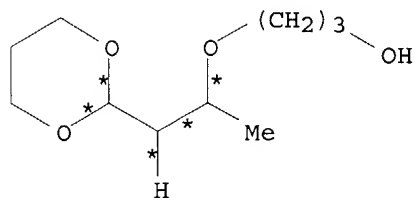
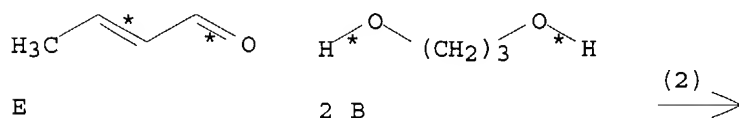
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The unsatd. cyclic acetal, 2-(1-propenyl)-1,3-dioxolane, was an  
intermediate in the 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H-catalyzed reaction of 2-butenal with  
excess ethylene glycol. The final product was 2-[2-(2-  
hydroxyethoxy)propyl]-1,3-dioxolane, and a small amount of cis- and  
trans-5-(2-hydroxyethoxy)-7-methyl-1,4-dioxepane.

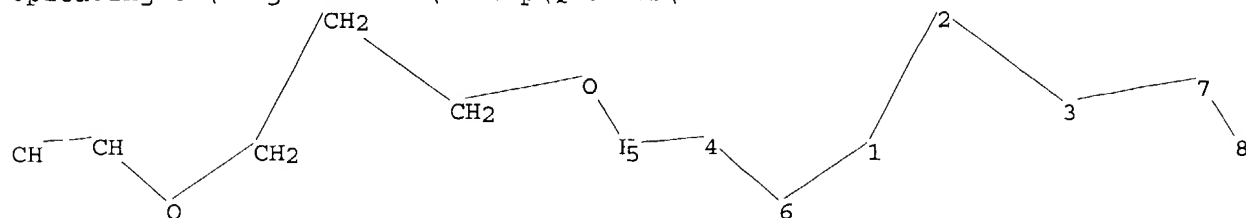
RX(2) OF 8 E + 2 B ==> F



F

RX(2) RCT E 4170-30-3, B 504-63-2  
PRO F 96424-48-5  
CAT 104-15-4 TsOH

>  
Uploading C:\Program Files\Stnexp\Queries\679174.str



chain nodes :

1 2 3 4 5 6 7 8

chain bonds :

1-2 1-6 2-3 3-7 4-5 4-6 7-8

exact/norm bonds :

4-6

exact bonds :

1-2 1-6 2-3 3-7 4-5 7-8

Match level :

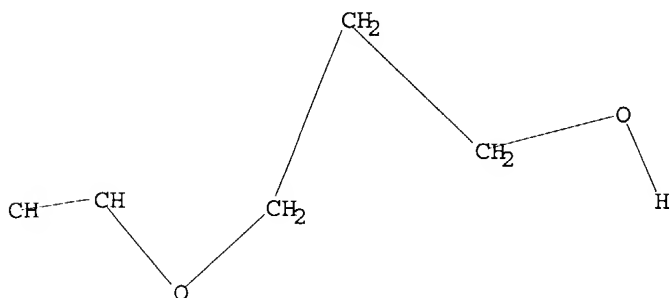
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 15:34:13 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 21528 TO ITERATE

4.6% PROCESSED 1000 ITERATIONS

5 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 421786 TO 439334

PROJECTED ANSWERS: 1530 TO 2774

L5 5 SEA SSS SAM L4

=> s his

L6 11725 HIS

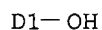
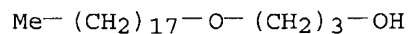
=> d scan l5

L5 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Propanediol, 3-(octadecyloxy)- (9CI)

MF C21 H44 O3

CI IDS



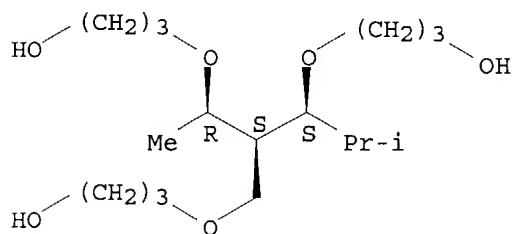
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L5 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1-Propanol, 3,3'-[[2-[1-(3-hydroxypropoxy)ethyl]-1-(1-methylethyl)-1,3-propanediyl]bis(oxy)]bis-, [1S-[1R\*,2R\*(S\*)]]- (9CI)

MF C17 H36 O6

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

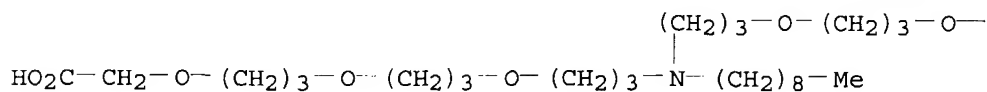
L5 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 3,7,11,19,23-Pentaoxa-15-azahexacosanoic acid, 26-hydroxy-15-nonyl-, sodium salt, compd. with N-p-hexylbenzoyl-N-methyltaurine (6CI)

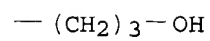
MF C29 H59 N O8 . C16 H25 N O4 S . Na

CM 1

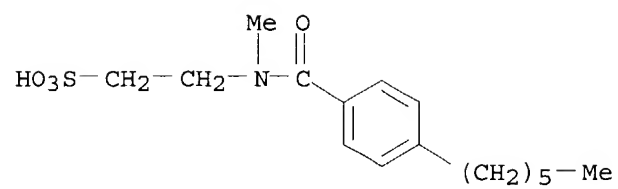
PAGE 1-A







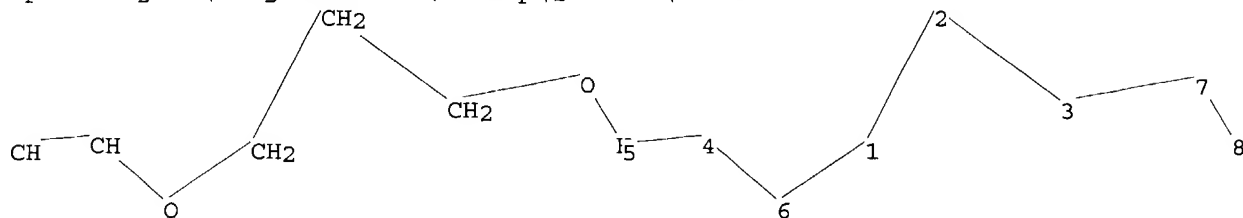
CM 2



\*\*\*\*\*

=>

Uploading C:\Program Files\Stnexp\Queries\679174.str



chain nodes :

1 2 3 4 5 6 7 8

chain bonds :

1-2 1-6 2-3 3-7 4-5 4-6 7-8

exact/norm bonds :

4-6

exact bonds :

1-2 1-6 2-3 3-7 4-5 7-8

Match level :

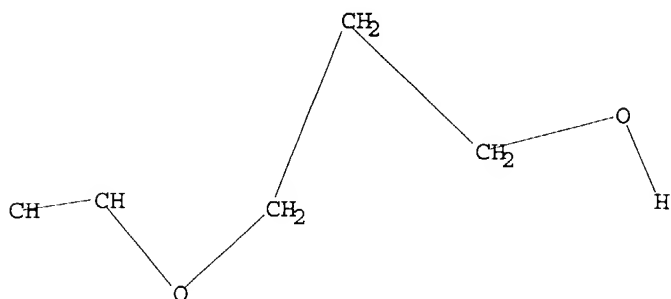
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 2/o not n/els

1796054 2/O

5757375 N/ELS

L4 617733 2/O NOT N/ELS

=> s l4 not (s/els or x/els or m/els)

1840876 S/ELS

0 X/ELS

0 M/ELS

L5 526528 L4 NOT (S/ELS OR X/ELS OR M/ELS)

=> s l5 not pms/ci

'CI' IS NOT A VALID FIELD CODE

0 PMS/CI

L6 526528 L5 NOT PMS/CI

=> s l3 subset=15

MISSING OPERATOR L3 SUBSET-L5

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s l3 subset=15

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full

FULL SUBSET SEARCH INITIATED 17:55:28 FILE 'BEILSTEIN'

FULL SUBSET SCREEN SEARCH COMPLETED - 3915 TO ITERATE

100.0% PROCESSED 3915 ITERATIONS

46 ANSWERS

SEARCH TIME: 00.00.15

L7 46 SEA SUB=L5 SSS FUL L3

=> s l7 and 1-5/nr

'NR' IS NOT A VALID FIELD CODE

0 1-5/NR

L8 0 L7 AND 1-5/NR

=> s l7 and pheny?

2387182 PHENY?

L9 8 L7 AND PHENY?

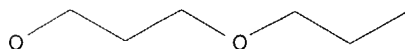
=> s l7 not l9

L10 38 L7 NOT L9

=> d ide 38

L10 ANSWER 38 OF 38 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	1697426
Beilstein Pref. RN (BPR):	4161-22-2
CAS Reg. No. (RN):	4161-22-2
Chemical Name (CN):	3-propoxy-propan-1-ol, trimethylene glycol-monopropyl ether
Autonom Name (AUN):	3-propoxy-propan-1-ol
Molec. Formula (MF):	C6 H14 O2
Molecular Weight (MW):	118.18
Lawson Number (LN):	523, 307
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	1486956
Tautomer ID (TAUTID):	1545775
Beilstein Citation (BSO):	1-01-00-00247, 4-01-00-02495, 5-01, 6-01
Entry Date (DED):	1989/02/27
Update Date (DUPD):	2000/02/29



Field Availability:

Code	Name	Occurrence
=====		

BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	2
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	4
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	7
CDER	Chemical Derivative	1
DEN	Density (Liquid)	2
FINFO	Further Information	1
LIQPH	Liquid Phase	1
MECM	Mechanical & Physical Property (MCS)	1
NMR	Nuclear Magnetic Resonance	1
RI	Refractive Index	3
SOUND	Acoustic Property	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	9
RXREA	Substance is Reaction Reactant	3
RXPRO	Substance is Reaction Product	6

=> s l10 and (isopro? or methylethyl or tertiary butyl )

276143 ISOPRO?

9515 METHYLETHYL

43 TERTIARY

561238 BUTYL

7 TERTIARY BUTYL

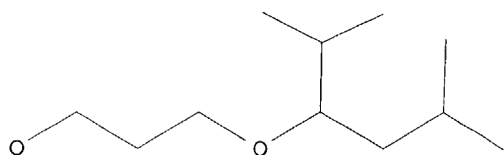
(TERTIARY(W) BUTYL)

L11 2 L10 AND (ISOPRO? OR METHYLETHYL OR TERTIARY BUTYL )

=> d ide 1-2

L11 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	6716050
Chemical Name (CN):	3-(1-isopropyl-3-methyl-butoxy) - propan-1-ol
Autonom Name (AUN):	3-(1-isopropyl-3-methyl-butoxy) - propan-1-ol
Molec. Formula (MF):	C11 H24 O2
Molecular Weight (MW):	188.31
Lawson Number (LN):	523, 347
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	5799856
Tautomer ID (TAUTID):	6354447
Beilstein Citation (BSO):	6-01
Entry Date (DED):	1994/07/18
Update Date (DUPD):	1994/07/18



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
DEN	Density (Liquid)	1
NMR	Nuclear Magnetic Resonance	1
RI	Refractive Index	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

L11 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 1732698  
 Beilstein Pref. RN (BPR): 110-48-5  
 CAS Reg. No. (RN): 110-48-5  
 Chemical Name (CN): **3-isopropoxy-propan-1-ol**  
 Autonom Name (AUN): **3-isopropoxy-propan-1-ol**  
 Molec. Formula (MF): C6 H14 O2  
 Molecular Weight (MW): 118.18  
 Lawson Number (LN): 523, 308  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 1568042  
 Tautomer ID (TAUTID): 1643021  
 Beilstein Citation (BSO): 4-01-00-02495, 5-01  
 Entry Date (DED): 1989/02/27  
 Update Date (DUPD): 1997/12/03



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	2
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	3
CDER	Chemical Derivative	1
RI	Refractive Index	2
XREF	Crossfile Reference	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	2

=> d frxpro 1

L11 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 1754057  
 Reactant BRN (.RBRN): 1340707, 3535134  
 Reactant (.RCT): 2-isopropyl-<1,3>dioxane,  
 isobutylmagnesium bromide  
 Product BRN (.PBRN): 6716050  
 Product (.PRO): 3-(1-isopropyl-3-methyl-butoxy)-propan-1-

ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 1754057.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 80 percent (BRN=6716050)  
Solvent (.SOL): diethyl ether  
Time (.TIM): 15 min  
Other Conditions (.COND): Heating  
Reference(s):  
1. Mel'nitskii, I. A.; Glukhova, O. F.; Kiladze, T. K.; Kantor, E. A.;  
Rakhmankulov, D. L.; Paushkin, Ya. M., Dokl.Chem.(Engl.Transl.), CODEN:  
DKCHAY, 292, <1987>, 83-84, Dokl.Akad.Nauk SSSR Ser.Khim., CODEN:  
DASKAJ, 292(6), <1987>, 1390-1392; BABS-5868508

=> d frxpro 2

L11 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 6949345  
Product BRN (.PBRN): 1732698  
Product (.PRO): 3-isopropoxy-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 6949345.1  
Reaction Classification (.CL): Preparation (half reaction)  
Reference(s):  
1. Smith; Williams, J.Amer.Chem.Soc., CODEN: JACSAT, 91, <1969>, 5254,5259

Reaction:

RX

Reaction ID (.ID): 3366  
Reactant BRN (.RBRN): 102382, 635639  
Reactant (.RCT): oxetane, propan-2-ol  
Product BRN (.PBRN): 1732698  
Product (.PRO): 3-isopropoxy-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 3366.1  
Reaction Classification (.CL): Preparation  
Other Conditions (.COND): 1731204  
Note(s) (.COM): Handbook  
Reference(s):  
1. Searles; Butler, J.Amer.Chem.Soc., CODEN: JACSAT, 76, <1954>, 56

=> d his

(FILE 'HOME' ENTERED AT 17:48:46 ON 15 APR 2004)

FILE 'REGISTRY' ENTERED AT 17:48:53 ON 15 APR 2004

L1 54830 S 3-PROPANEDIOL

L2 10 S 3-PROPANEDIOL AND C3H8O2/MF

UPD	Update Date	1
BP	Boiling Point	1
IR	Infrared Spectrum	1
PHARM	Pharmacological Data	1
RI	Refractive Index	2
XREF	Crossfile Reference	1

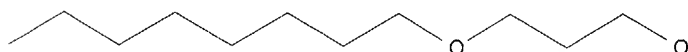
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	2

=> d ide l12 12

L12 ANSWER 12 OF 36 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6185575  
 Chemical Name (CN): 3-octyloxypropan-1-ol  
 Autonom Name (AUN): 3-octyloxy-propan-1-ol  
 Molec. Formula (MF): C11 H24 O2  
 Molecular Weight (MW): 188.31  
 Lawson Number (LN): 523, 344  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 5335889  
 Tautomer ID (TAUTID): 5806321  
 Beilstein Citation (BSO): 6-01  
 Entry Date (DED): 1993/10/20  
 Update Date (DUPD): 1995/05/11



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
------	------	------------



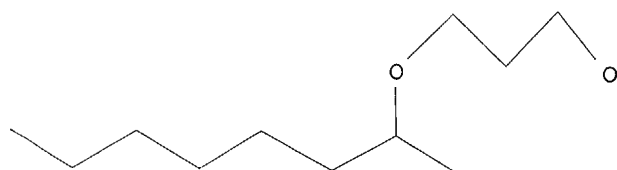
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=====
RX          Reaction Documents                2
RXPRO       Substance is Reaction Product     2
```

=> s l12 and methyl?  
 2664228 METHYL?  
 L14 7 L12 AND METHYL?

=> d ide 7

L14 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

```
Beilstein Records (BRN):      4304771
Chemical Name (CN):           3-(1-methyl-heptyloxy)-propan-1-ol
Autonom Name (AUN):           3-(1-methyl-heptyloxy)-propan-1-ol
Molec. Formula (MF):          C11 H24 O2
Molecular Weight (MW):        188.31
Lawson Number (LN):           523, 345
Compound Type (CTYPE):        acyclic
Constitution ID (CONSID):      3888340
Tautomer ID (TAUTID):         4144953
Beilstein Citation (BSO):      6-01
Entry Date (DED):             1992/07/20
Update Date (DUPD):           1992/09/22
```



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d frxpro 7

L14 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID):	1537307
Reactant BRN (.RBRN):	106557
Reactant (.RCT):	2-hexyl-2-methyl-<1,3>dioxane
Product BRN (.PBRN):	4304771
Product (.PRO):	3-(1-methyl-heptyloxy)-propan-1-ol
No. of React. Details (.NVAR):	1

Reaction Details:

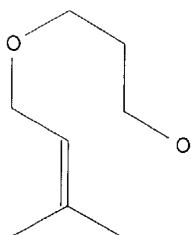
RX

Reaction RID (.RID):	1537307.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	53 percent (BRN=4304771)
Reagent (.RGT):	trimethylsilyl trifluoromethanesulphonate (TMSOTf), BH3S*Me2
Solvent (.SOL):	CH2Cl2
Temperature (.T):	-78 Cel
Reference(s):	1. Hunter, Roger; Bartels, Birgit; Michael, Joseph P., Tetrahedron Lett., CODEN: TELEAY, 32(8), <1991>, 1095-1098; BABS-5539910

=> d 6

L14 ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	5917293
Beilstein Pref. RN (BPR):	126274-83-7
CAS Reg. No. (RN):	126274-83-7
Chemical Name (CN):	7-methyl-4-oxa-6-octen-1-ol
Autonom Name (AUN):	3-(3-methyl-but-2-enyloxy)-propan-1-ol
Molec. Formula (MF):	C8 H16 O2
Molecular Weight (MW):	144.21
Lawson Number (LN):	523, 422
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	5162765
Tautomer ID (TAUTID):	5614415
Beilstein Citation (BSO):	6-01
Entry Date (DED):	1993/07/22
Update Date (DUPD):	1997/08/11



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	2
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4

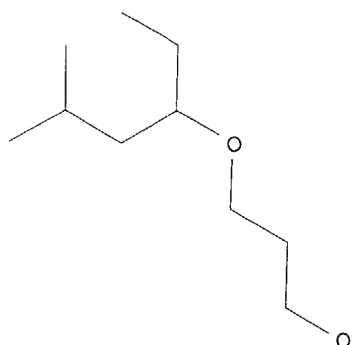
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d 5

L14 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6185309  
 Chemical Name (CN): 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol  
 Autonom Name (AUN): 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol  
 Molec. Formula (MF): C10 H22 O2  
 Molecular Weight (MW): 174.28  
 Lawson Number (LN): 523, 337  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 5324570  
 Tautomer ID (TAUTID): 5800315  
 Beilstein Citation (BSO): 6-01  
 Entry Date (DED): 1993/10/20  
 Update Date (DUPD): 1994/10/31



Field Availability:

Code	Name	Occurrence
=====	=====	=====
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	2
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3
RI	Refractive Index	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	3
RXPRO	Substance is Reaction Product	3

=> d frxpro 5

L14 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 1513740  
 Reactant BRN (.RBRN): 103967  
 Reactant (.RCT): 2-isobutyl-<1,3>dioxane  
 Product BRN (.PBRN): 6185309, 6715910  
 Product (.PRO): 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol,  
 3-(3-methyl-butoxy)-propan-1-ol  
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 1513740.1  
 Reaction Classification (.CL): Preparation

Yield (.YDT): 0.02 mol (BRN=6185309), 0.02 mol  
(BRN=6715910)  
Reagent (.RGT): diethylaluminum hydride, triethylaluminum  
Solvent (.SOL): kerosene, hexane  
Time (.TIM): 15 hour(s)  
Other Conditions (.COND): Heating  
Reference(s):  
1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L.,  
J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423,  
Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552;  
BABS-5880479

Reaction:

RX

Reaction ID (.ID): 1513739  
Reactant BRN (.RBRN): 103967, 3587229  
Reactant (.RCT): 2-isobutyl-<1,3>dioxane, triethylaluminium  
Product BRN (.PBRN): 6715910, 6185309  
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol,  
3-(1-ethyl-3-methyl-butoxy)-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 1513739.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 0.01 mol (BRN=6715910), 0.035 mol  
(BRN=6185309)  
Reagent (.RGT): diethylaluminum hydride  
Solvent (.SOL): kerosene, hexane  
Time (.TIM): 30 hour(s)  
Other Conditions (.COND): Heating  
Reference(s):  
1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L.,  
J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423,  
Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552;  
BABS-5880479

Reaction:

RX

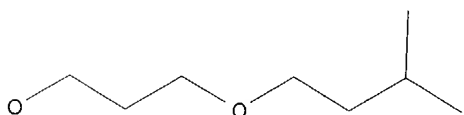
Reaction ID (.ID): 1513738  
Reactant BRN (.RBRN): 103967, 3587229  
Reactant (.RCT): 2-isobutyl-<1,3>dioxane, triethylaluminium  
Product BRN (.PBRN): 6185309  
Product (.PRO): 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 1513738.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 68 percent (BRN=6185309)  
Solvent (.SOL): hexane  
Time (.TIM): 5 min  
Temperature (.T): 70 Cel  
Reference(s):  
1. Volkov, A. A.; Zlotskii, S. S.; Kravets, E. Kh; Rakhmankulov, D. L.,  
Dokl.Chem.(Engl.Transl.), CODEN: DKCHAY, 283, <1985>, 246-248,  
Dokl.Akad.Nauk SSSR Ser.Khim., CODEN: DASKAJ, 283(5), <1985>,  
1194-1196; BABS-5773191

Beilstein Records (BRN): 6715910  
 Chemical Name (CN): 3-(3-methyl-butoxy)-propan-1-ol  
 Autonom Name (AUN): 3-(3-methyl-butoxy)-propan-1-ol  
 Molec. Formula (MF): C8 H18 O2  
 Molecular Weight (MW): 146.23  
 Lawson Number (LN): 523, 326  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 5798151  
 Tautomer ID (TAUTID): 6353156  
 Beilstein Citation (BSO): 6-01  
 Entry Date (DED): 1994/07/18  
 Update Date (DUPD): 1998/11/09



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	1
DEN	Density (Liquid)	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	2
RI	Refractive Index	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	4
RXPRO	Substance is Reaction Product	4

=> d frxpro 4

Reaction:

RX

Reaction ID (.ID): 4855860

Reactant BRN (.RBRN): 3535405, 102532  
Reactant (.RCT): isobutylmagnesium bromide, <1,3>dioxane  
Product BRN (.PBRN): 6715910  
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 4855860.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 40 percent (BRN=6715910)  
Reagent (.RGT): ZnBr2  
Solvent (.SOL): diethyl ether  
Time (.TIM): 2 hour(s)  
Other Conditions (.COND): Heating  
Reference(s):  
1. Sunagatov, M. F.; Mel'nitskii, L. A.; Kantor, E. A., Russ.J.Gen.Chem., CODEN: RJGCEK, 67(2), <1997>, 270-272, Zh.Obshch.Khim., CODEN: ZOKHA4, 67(2), <1997>, 288-290; BABS-6089219

Reaction:

RX

Reaction ID (.ID): 1513740  
Reactant BRN (.RBRN): 103967  
Reactant (.RCT): 2-isobutyl-<1,3>dioxane  
Product BRN (.PBRN): 6185309, 6715910  
Product (.PRO): 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol,  
3-(3-methyl-butoxy)-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 1513740.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 0.02 mol (BRN=6185309), 0.02 mol  
(BRN=6715910)  
Reagent (.RGT): diethylaluminum hydride, triethylaluminum  
Solvent (.SOL): kerosene, hexane  
Time (.TIM): 15 hour(s)  
Other Conditions (.COND): Heating  
Reference(s):  
1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552; BABS-5880479

Reaction:

RX

Reaction ID (.ID): 1513739  
Reactant BRN (.RBRN): 103967, 3587229  
Reactant (.RCT): 2-isobutyl-<1,3>dioxane, triethylaluminium  
Product BRN (.PBRN): 6715910, 6185309  
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol,  
3-(1-ethyl-3-methyl-butoxy)-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 1513739.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 0.01 mol (BRN=6715910), 0.035 mol  
(BRN=6185309)  
Reagent (.RGT): diethylaluminum hydride  
Solvent (.SOL): kerosene, hexane

Time (.TIM): 30 hour(s)

Other Conditions (.COND): Heating

Reference(s):

1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552; BABS-5880479

Reaction:

RX

Reaction ID (.ID): 1488274  
Reactant BRN (.RBRN): 102532, 3535134  
Reactant (.RCT): <1,3>dioxane, isobutylmagnesium bromide  
Product BRN (.PBRN): 6715910  
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 1488274.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 73 percent (BRN=6715910)  
Solvent (.SOL): diethyl ether  
Time (.TIM): 15 min  
Other Conditions (.COND): Heating  
Reference(s):  
1. Mel'nitskii, I. A.; Glukhova, O. F.; Kiladze, T. K.; Kantor, E. A.; Rakhmankulov, D. L.; Paushkin, Ya. M., Dokl.Chem.(Engl.Transl.), CODEN: DKCHAY, 292, <1987>, 83-84, Dokl.Akad.Nauk SSSR Ser.Khim., CODEN: DASKAJ, 292(6), <1987>, 1390-1392; BABS-5868508

=> d frxpro 3 ide

L14 ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 3662167  
Reactant BRN (.RBRN): 6720068  
Reactant (.RCT): 3-<3-(hexyl-methyl-silanyl)-propoxy>-propionic acid methyl ester  
Product BRN (.PBRN): 6716507  
Product (.PRO): 3-<3-(hexylmethyilsilyl)propoxy>-1-propanol  
No. of React. Details (.NVAR): 1

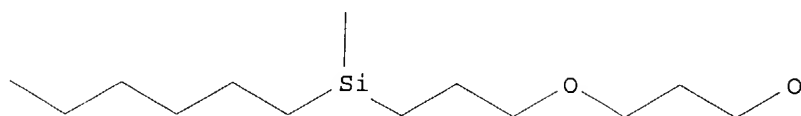
Reaction Details:

RX

Reaction RID (.RID): 3662167.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 72 percent (BRN=6716507)  
Reagent (.RGT): LiAlH4  
Solvent (.SOL): diethyl ether  
Time (.TIM): 10 hour(s)  
Temperature (.T): 20 Cel  
Reference(s):  
1. Sultanov, R. A.; Gazarov, T. Sh.; Saryev, G. A., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 54, <1984>, 1005-1007, Zh.Obshch.Khim., CODEN: ZOKHA4, 54(5), <1984>, 1122-1125; BABS-5871217  
Beilstein Records (BRN): 6716507  
Chemical Name (CN): 3-<3-(hexylmethyilsilyl)propoxy>-1-propanol  
Autonom Name (AUN): 3-<3-(hexyl-methyl-silanyl)-propoxy>-propan-1-ol



Molec. Formula (MF): C13 H30 O2 Si  
 Molecular Weight (MW): 246.46  
 Lawson Number (LN): 3803, 3798, 3777, 523  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 5818489  
 Tautomer ID (TAUTID): 6367435  
 Beilstein Citation (BSO): 6-04  
 Entry Date (DED): 1994/07/18  
 Update Date (DUPD): 1994/07/19



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	1
DEN	Density (Liquid)	1
IR	Infrared Spectrum	1
RI	Refractive Index	1

This substance also occurs in Reaction Documents:

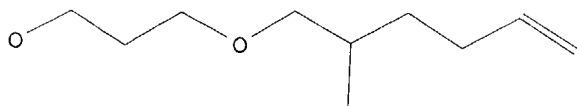
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d ide 2

L14 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7914336  
 Chemical Name (CN): 3-(2-methyl-hex-5-enyloxy)-propan-1-ol  
 Autonom Name (AUN): 3-(2-methyl-hex-5-enyloxy)-propan-1-ol  
 Molec. Formula (MF): C10 H20 O2  
 Molecular Weight (MW): 172.27  
 Lawson Number (LN): 523, 432  
 Compound Type (CTYPE): acyclic  
 Constitution ID (CONSID): 6749116

Tautomer ID (TAUTID): 7484361  
 Beilstein Citation (BSO): 6-01  
 Entry Date (DED): 1998/11/09  
 Update Date (DUPD): 1998/11/09



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

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L14 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 4870816  
 Reactant BRN (.RBRN): 3587197, 2071854  
 Reactant (.RCT): trimethylaluminium, 3-allyloxy-propan-1-ol  
 Product BRN (.PBRN): 969155, 7914336  
 Product (.PRO): propane-1,3-diol, 3-(2-methyl-hex-5-enyloxy)-propan-1-ol  
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

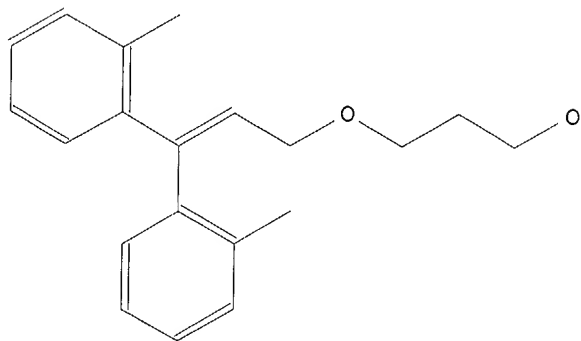
Reaction RID (.RID): 4870816.1  
 Reaction Classification (.CL): Preparation  
 Yield (.YDT): 27 percent (BRN=7914336)  
 Catalyst (.CAT): (dppp)NiCl2  
 Solvent (.SOL): toluene  
 Reference(s):  
 1. Taniguchi, Takahiko; Ogasawara, Kunio, Chem.Comm., CODEN: CHCOFS(15),

<1998>, 1531-1532; BABS-6094785

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L14 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 8496244  
Chemical Name (CN): 3-((-bis(2-methylphenyl)-1-propen-3-yl)oxy)-1-propanol  
Autonom Name (AUN): 3-(3,3-di-o-tolyl-allyloxy)-propan-1-ol  
Molec. Formula (MF): C20 H24 O2  
Molecular Weight (MW): 296.41  
Lawson Number (LN): 5590, 523  
Compound Type (CTYPE): isocyclic  
Constitution ID (CONSID): 7203783  
Tautomer ID (TAUTID): 7990827  
Entry Date (DED): 2000/07/18  
Update Date (DUPD): 2000/07/18



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

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L14 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID):	8536350
Reactant BRN (.RBRN):	969155, 8486168
Reactant (.RCT):	propane-1,3-diol, 3-bromo-1,1-bis(2-methylphenyl)-1-propene
Product BRN (.PBRN):	8496244
Product (.PRO):	3-(3,3-di-o-tolyl-allyloxy)-propan-1-ol
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	8536350.1
Reaction Classification (.CL):	Multistage
Yield (.YDT):	31 percent (BRN=8496244)
Nr. of Stages (.SNR):	2
Stage 1	
Reagent (.RGT):	nBuLi
Solvent (.SOL):	hexane
Time (.TIM):	0.5 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Metallation
Stage 2	
Stage reactant (.SRCT):	3-bromo-1,1-bis(2-methylphenyl)-1-propene
Stage Reactant BRN (.SRBRN):	8486168
Solvent (.SOL):	hexane
Time (.TIM):	36 hour(s)
Temperature (.T):	75 Cel
Reaction Type (.TYP):	Etherification
Reference(s):	

1. Andersen, Knud Erik; Soerensen, Jan L.; Huusfeldt, Per O.; Knutsen, Lars J. S.; Lau, Jesper; Lundt, Behrend F.; Petersen, Hans; Suzdak, Peter D.; Swedberg, Michael D. B., J.Med.Chem., CODEN: JMCMAR, 42(21), <1999>, 4281 - 4291; BABS-6228258

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